

# 1,3,6,8-Tetranitrocarbazole

<b>Other names:</b>	9H-Carbazole, 1,3,6,8-tetranitro-Carbazole, 1,3,6,8-tetranitro-Nirosan TNC
<b>Inchi:</b>	InChI=1S/C12H5N5O8/c18-14(19)5-1-7-8-2-6(15(20)21)4-10(17(24)25)12(8)13-11(7)9(3
<b>InchiKey:</b>	JUSWGNJYSBSOFM-UHFFFAOYSA-N
<b>Formula:</b>	C12H5N5O8
<b>SMILES:</b>	O=[N+]([O-])c1cc([N+](=O)[O-])c2[nH]c3c([N+](=O)[O-])cc([N+](=O)[O-])cc3c2c1
<b>Mol. weight [g/mol]:</b>	347.20
<b>CAS:</b>	4543-33-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.90		Crippen Method
logp	2.472		Crippen Method
mcvol	201.220	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4543333&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4543333&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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